# CPSC 330 Applied Machine Learning

# Lecture 13: Feature engineering and feature selection

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# **Imports**

```
In [1]:
            import os
           import sys
         4 import matplotlib.pyplot as plt
         5 import numpy as np
         6 import numpy.random as npr
         7 import pandas as pd
         8 from sklearn.compose import (
                ColumnTransformer,
        10
                TransformedTargetRegressor,
        11
                make column transformer,
        12 )
        13 from sklearn.dummy import DummyRegressor
        14 from sklearn.ensemble import RandomForestRegressor
        15 from sklearn.impute import SimpleImputer
        16 from sklearn.linear model import LinearRegression, LogisticRegression,
        17 from sklearn.metrics import make scorer, mean squared error, r2 score
        18 from sklearn.model selection import cross val score, cross validate, tr
        19 from sklearn.pipeline import Pipeline, make pipeline
        20 from sklearn.preprocessing import OneHotEncoder, OrdinalEncoder, Standa
        21 from sklearn.svm import SVC
        22 from sklearn.tree import DecisionTreeRegressor
```

```
In [3]: 1 import sys
2 sys.path.append("../code/.")
```

# Learning outcomes

From this lecture, students are expected to be able to:

 Explain what feature engineering is and the importance of feature engineering in building machine learning models.

- · Carry out preliminary feature engineering on text data.
- Explain the general concept of feature selection.
- Discuss and compare different feature selection methods at a high level.
- Use sklearn's implementation of recursive feature elimination (RFE) and forward and backward selection (SequentialFeatureSelector).

# **Feature engineering: Motivation**

# What is feature engineering?

- Better features: more flexibility, higher score, we can get by with simple and more interpretable models.
- If your features, i.e., representation is bad, whatever fancier model you build is not going to help ("garbage in, garbage out"). This is less true now with deep learning.

**Feature engineering** is the process of transforming raw data into features that better represent the underlying problem to the predictive models, resulting in improved model accuracy on unseen data.

- Jason Brownlee

# Some quotes on feature engineering

A quote by Pedro Domingos <u>A Few Useful Things to Know About Machine Learning</u> (<a href="https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf">https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf</a>)

... At the end of the day, some machine learning projects succeed and some fail. What makes the difference? Easily the most important factor is the features used.

A quote by Andrew Ng, <u>Machine Learning and AI via Brain simulations</u> (https://ai.stanford.edu/~ang/slides/DeepLearning-Mar2013.pptx)

Coming up with features is difficult, time-consuming, requires expert knowledge. "Applied machine learning" is basically feature engineering.

# Better features usually help more than a better model.

- Good features would ideally:
  - capture most important aspects of the problem
  - allow learning with few examples
  - generalize to new scenarios.
- There is a trade-off between simple and expressive features:
  - With simple features overfitting risk is low, but scores might be low.

With complicated features scores can be high, but so is overfitting risk.

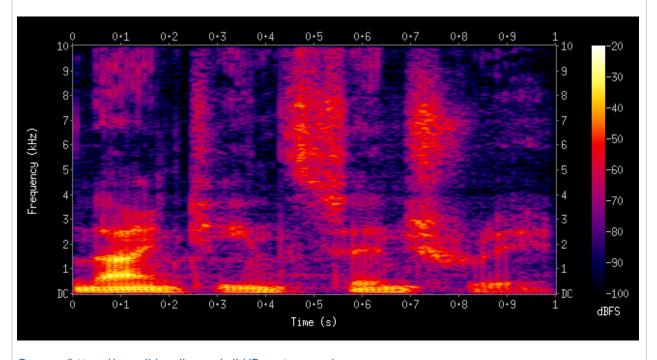
# The best features may be dependent on the model you use.

- Examples:
  - For counting-based methods like decision trees separate relevant groups of variable values
    - Discretization makes sense
  - For distance-based methods like KNN, we want different class labels to be "far".
    - Standardization
  - For regression-based methods like linear regression, we want targets to have a linear dependency on features.

### **Domain-specific transformations**

In some domains there are natural transformations to do:

- Spectrograms (sound data)
- · Wavelets (image data)
- Convolutions



Source (https://en.wikipedia.org/wiki/Spectrogram)

In this lecture, I'll show you two example domains where feature engineering plays an important role:

- · Text data
- Audio data

# Common features used in text classification

# **Bag of words**

- So far for text data we have been using bag of word features.
- They are good enough for many tasks. But ...
- This encoding throws out a lot of things we know about language
- It assumes that word order is not that important.
- So if you want to improve the scores further on text classification tasks you carry out feature engineering.

Let's look at some examples from research papers.

# **Example: Label "Personalized" Important E-mails:**

- The Learning Behind Gmail Priority Inbox (<a href="https://static.googleusercontent.com/media/research.google.com/en//pubs/archive/36955.pdf">https://static.googleusercontent.com/media/research.google.com/en//pubs/archive/36955.pdf</a>)
- Features: bag of words, trigrams, regular expressions, and so on.
- There might be some "globally" important messages:
  - "This is your mother, something terrible happened, give me a call ASAP."
- But your "important" message may be unimportant to others.
  - Similar for spam: "spam" for one user could be "not spam" for another.
- Social features (e.g., percentage of sender emails that is read by the recipient)
- Content features (e.g., recent terms the user has been using in emails)
- Thread features (e.g., whether the user has started the thread)
- ...

# **The Learning Behind Gmail Priority Inbox**

# (https://static.googleusercontent.com/media/research.google.com/en//pr

### 2.1 Features

Feature engineering examples: <u>Automatically Identifying Good Conversations Online (http://www.courtneynapoles.com/res/icwsm17-automatically.pdf)</u>

BOW	Counts of tokens.
(21k)	
Embeddings	Averaged word embedding values from Google
(300)	News vectors (Mikolov et al. 2013).
Entity (12)	Counts of named entity types.
Length (2)	Mean # sentences/comment, # tokens/sentence.
Lexicon (6)	# pronouns; agreement and certainty phrases;
	discourse connectives; and abusive language.
<b>POS</b> (23 <i>k</i> )	Counts of 1–3-gram POS tags.
Popularity	# thumbs up (TU), # thumbs down (TD), TU +
(4)	TD, and $\frac{TU}{TU+TD}$ .
Similarity	Overlap between comment and headline, first
(8)	comment, previous comment, and all previous
	comments (if applicable).
User (7)	# comments posted, # threads participated in, #
	threads initiated, TU and TD received, and com-
	menting rate.

Table 4: Features used in the linear model. The number of features from each group is indicated in parentheses.

# (optional) Term weighing (TF-IDF)

- A measure of relatedness between words and documents
- Intuition: Meaningful words may occur repeatedly in related documents, but functional words (e.g., *make*, *the*) may be distributed evenly over all documents

$$tf.idf(w_i, d_j) = (1 + log(tf_{ij}))log\frac{D}{df_i}$$

### where,

- $\operatorname{tf}_{ij} o (\operatorname{term} \operatorname{frequency})$  number of occurrences of the  $\operatorname{term} w_i$  in document  $d_j$
- $D \rightarrow$  number of documents
- $df_i \rightarrow (document frequency)$  number of documents in which  $w_i$  occurs

Check TfidfVectorizer from sklearn.

# **N**-grams

- · Incorporating more context
- A contiguous sequence of *n* items (characters, tokens) in text.

CPSC330 students are hard-working.

- 2-grams (bigrams): a contiguous sequence of two words
  - CPSC330 students, students are, are hard-working.
- · 3-grams (trigrams): a contiguous sequence of three words
  - CPSC330 students are, students are hard-working.

You can extract ngram features using CountVectorizer by passing ngram\_range.

```
In [2]:
            from sklearn.feature_extraction.text import CountVectorizer
         1
          2
          3
            X = [
                 "URGENT!! As a valued network customer you have been selected to re
          4
          5
                "Lol you are always so convincing.",
                "URGENT!! Call right away!!",
          6
          7
            vec = CountVectorizer(ngram range=(1, 3))
            X_counts = vec.fit_transform(X)
         10 bow df = pd.DataFrame(X counts.toarray(), columns=vec.get feature names
```

In [3]: 1 bow\_df

### Out[3]:

	900	900 prize	900 prize reward	always	always so	always so convincing	are	are always	are always so	as	 urgent call	uı
URGENT!! As a valued network customer you have been selected to receive a \$900 prize reward!	1	1	1	0	0	0	0	0	0	1	 0	
Lol you are always so convincing.	0	0	0	1	1	1	1	1	1	0	 0	
URGENT!! Call right away!!	0	0	0	0	0	0	0	0	0	0	 1	

3 rows × 61 columns

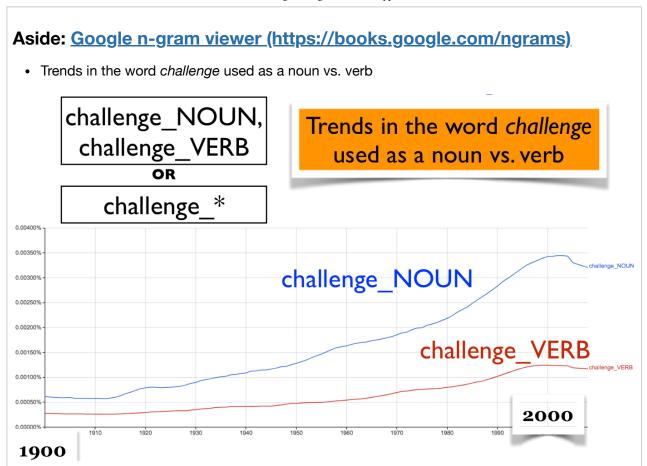
# ASIDE: Google n-gram viewer (https://books.google.com/ngrams)

- · All Our N-gram are Belong to You
  - https://ai.googleblog.com/2006/08/all-our-n-gram-are-belong-toyou.html (https://ai.googleblog.com/2006/08/all-our-n-gram-are-belong-toyou.html)

Here at Google Research we have been using word n-gram models for a variety of R&D projects, such as statistical machine translation, speech recognition, spelling correction, entity detection, information extraction, and others. That's why we decided to share this enormous dataset with everyone. We processed 1,024,908,267,229 words of running text and are publishing the counts for all 1,176,470,663 five-word sequences that appear at least 40 times. There are 13,588,391 unique words, after discarding words that appear less than 200 times."

### Out[4]:

# Aside: Google n-gram viewer (https://books.google.com/ngrams) • Count the occurrences of the bigram smart women in the corpus from 1900 to 2000 How often does smart association corpus modify women in American women=>smart:eng\_us\_2012, women=>smart:eng gb 2012 vs British English? women⇒smart:eng gb 2012 women=>smart:eng us 2012 0.000004509 0.00000350% 0.000002509 0.00000150% 0.000000509 0.00000000% 1980



# Part-of-speech features

### Part-of-speech (POS) in English

- Part-of-speech: A kind of syntactic category that tells you some of the grammatical properties
  of a word.
  - Noun → water, sun, cat
  - Verb → run, eat, teach

The \_\_\_\_ was running.

· Only a noun fits here.

# Part-of-speech (POS) features

• POS features use POS information for the words in text.

CPSC330/PROPER\_NOUN students/NOUN are/VERB hard-working/ADJECTIVE

# An example from a project

- · Data: a bunch of documents
- Task: identify texts with *permissions* and identify who is giving permission to whom.

**You** may **disclose** Google confidential information when compelled to do so by law if **you** provide **us** reasonable prior notice, unless a court orders that **we** not receive notice.

- · A very simple solution
  - Look for pronouns and verbs.
  - Add POS tags as features in your model.
  - Maybe look up words similar to disclose.

# Penn Treebank part-of-speech tags (bonus)

Tag	Description	Example	Tag	Description	Example	Tag	Description	Example
CC	coordinating	and, but, or	PDT	predeterminer	all, both	VBP	verb non-3sg	eat
	conjunction						present	
CD	cardinal number	one, two	POS	possessive ending	's	VBZ	verb 3sg pres	eats
DT	determiner	a, the	PRP	personal pronoun	I, you, he	WDT	wh-determ.	which, that
EX	existential 'there'	there	PRP\$	possess. pronoun	your, one's	WP	wh-pronoun	what, who
FW	foreign word	mea culpa	RB	adverb	quickly	WP\$	wh-possess.	whose
IN	preposition/	of, in, by	RBR	comparative	faster	WRB	wh-adverb	how, where
	subordin-conj			adverb				
JJ	adjective	yellow	RBS	superlatv. adverb	fastest	\$	dollar sign	\$
JJR	comparative adj	bigger	RP	particle	up, off	#	pound sign	#
JJS	superlative adj	wildest	SYM	symbol	+,%, &	"	left quote	' or "
LS	list item marker	1, 2, One	TO	"to"	to	,,	right quote	' or "
MD	modal	can, should	UH	interjection	ah, oops	(	left paren	[, (, {, <
NN	sing or mass noun	llama	VB	verb base form	eat	)	right paren	], ), }, >
NNS	noun, plural	llamas	VBD	verb past tense	ate	,	comma	,
NNP	proper noun, sing.	<i>IBM</i>	VBG	verb gerund	eating		sent-end punc	.!?
NNPS	proper noun, plu.	Carolinas	VBN	verb past part.	eaten	:	sent-mid punc	: ;

- How do we extract part-of-speech information?
- We use pre-trained models!
- A couple of popular libraries which include such pre-trained models.
- nltk

conda install -c anaconda nltk

spaCy

conda install -c conda-forge spacy

```
In [5]: import nltk
2
3 nltk.download("punkt")

[nltk_data] Downloading package punkt to /Users/mathias/nltk_data...
[nltk_data] Package punkt is already up-to-date!
```

Out[5]: True

 You also need to download the language model which contains all the pre-trained models. For that run the following in your course conda environment.

```
In [6]: 1 # python -m spacy download en_core_web_md
```

# spaCy (https://spacy.io/)

A useful package for text processing and feature extraction

- Active development: <a href="https://github.com/explosion/spaCy">https://github.com/explosion/spaCy</a>
   (<a href="https://github.com/explosion/spaCy">https://github.com/explosion/spaCy</a>
- Interactive lessons by Ines Montani: <a href="https://course.spacy.io/en/">https://course.spacy.io/en/</a> (<a href="https://course.spacy.io/en/">https://course.spacy.io/en/</a> (<a href="https://course.spacy.io/en/">https://course.spacy.io/en/</a> (<a href="https://course.spacy.io/en/">https://course.spacy.io/en/</a> (<a href="https://course.spacy.io/en/">https://course.spacy.io/en/</a>)
- · Good documentation, easy to use, and customizable.

```
In [7]: import en_core_web_md # pre-trained model
import spacy
3
4 nlp = en_core_web_md.load()
```

```
In [8]:

1 sample_text = """Dolly Parton is a gift to us all.

2 From writing all-time great songs like "Jolene" and "I Will Always Love

3 to great performances in films like 9 to 5, to helping fund a COVID-19

4 she's given us so much. Now, Netflix bring us Dolly Parton's Christmas

5 an original musical that stars Christine Baranski as a Scrooge-like lan

6 who threatens to evict an entire town on Christmas Eve to make room for

7 Directed and choreographed by the legendary Debbie Allen and counting J

8 and Parton herself amongst its cast, Christmas on the Square seems like

9 to save Christmas 2020.

# [Adapted from here.](https://thepopbreak.com/2020/11/22/dolly-partons)
```

Spacy extracts all interesting information from text with this call.

```
In [9]: 1 doc = nlp(sample_text)
```

Let's look at part-of-speech tags.

```
In [10]: 1 print([(token, token.pos_) for token in doc][:20])
```

[(Dolly, 'PROPN'), (Parton, 'PROPN'), (is, 'AUX'), (a, 'DET'), (gift, 'NO
UN'), (to, 'ADP'), (us, 'PRON'), (all, 'PRON'), (., 'PUNCT'), (
, 'SPACE'), (From, 'ADP'), (writing, 'VERB'), (all, 'DET'), (-, 'PUNCT'),
(time, 'NOUN'), (great, 'ADJ'), (songs, 'NOUN'), (like, 'ADP'), (", 'PUNC
T'), (Jolene, 'PROPN')]

- Often we want to know who did what to whom.
- Named entities give you this information.
- · What are named entities in the text?

```
In [11]: 1 print("Named entities:\n", [(ent.text, ent.label_) for ent in doc.ents]
2 print("\nORG means: ", spacy.explain("ORG"))
3 print("\nPERSON means: ", spacy.explain("PERSON"))
4 print("\nDATE means: ", spacy.explain("DATE"))
```

```
Named entities:

[('Dolly Parton', 'PERSON'), ('Jolene', 'PERSON'), ('9 to 5', 'DATE'),

('Netflix', 'ORG'), ('Dolly Parton', 'PERSON'), ('Christmas', 'DATE'),

('Square', 'FAC'), ('Christine Baranski', 'PERSON'), ('Christmas Eve', 'D

ATE'), ('Debbie Allen', 'PERSON'), ('Jennifer Lewis', 'PERSON'), ('Parton', 'PERSON'), ('Christmas', 'DATE'), ('Square', 'FAC'), ('Christmas 2020', 'DATE')]
```

ORG means: Companies, agencies, institutions, etc.

PERSON means: People, including fictional

DATE means: Absolute or relative dates or periods

Dolly Parton **PERSON** is a gift to us all.

From writing all-time great songs like "Jolene PERSON" and "I Will Always Love You", to great performances in films like 9 to 5 DATE, to helping fund a COVID-19 vaccine, she's given us so much. Now, Netflix ORG bring us Dolly Parton PERSON's Christmas DATE on the Square FAC, an original musical that stars Christine Baranski PERSON as a Scrooge-like landowner who threatens to evict an entire town on Christmas Eve DATE to make room for a new mall.

Directed and choreographed by the legendary Debbie Allen **PERSON** and counting Jennifer

Lewis **PERSON** 

and Parton PERSON herself amongst its cast, Christmas DATE on the Square FAC seems like the perfect movie

to save Christmas 2020 DATE . 🐸 📥

# An example from a project

Goal: Extract and visualize inter-corporate relationships from disclosed annual 10-K reports of public companies.

Source for the text below. (https://www.bbc.com/news/business-39875417)

```
In [13]: 1 text = (
2    "Heavy hitters, including Microsoft and Google, "
3    "are competing for customers in cloud services with the likes of IB
4 )
```

Heavy hitters, including Microsoft org and Google org, are competing for customers in cloud services with the likes of IBM org and Salesforce PRODUCT.

```
Named entities:
 [('Microsoft', 'ORG'), ('Google', 'ORG'), ('IBM', 'ORG'), ('Salesforce',
'PRODUCT')]
```

If you want emoji identification support install spacymoji (https://pypi.org/project/spacymoji/) in the course environment.

```
pip install spacymoji
```

After installing <code>spacymoji</code>, if it's still complaining about module not found, my guess is that you do not have <code>pip</code> installed in your <code>conda</code> environment. Go to your course <code>conda</code> environment install <code>pip</code> and install the <code>spacymoji</code> package in the environment using the <code>pip</code> you just installed in the current environment.

```
conda install pip
YOUR_MINICONDA_PATH/miniconda3/envs/cpsc330/bin/pip install spacymo
ji
```

Does the text have any emojis? If yes, extract the description.

### **Final remarks**

- If we want to go beyond bag-of-words and incorporate human knowledge in models, we carry out feature engineering.
- Some common features include:
  - ngram features
  - part-of-speech features
  - named entity features
  - emoticons in text
- These are usually extracted from pre-trained models using libraries such as spaCy.
- · Now a lot of this has moved to deep learning.
- But industries still rely on manual feature engineering.

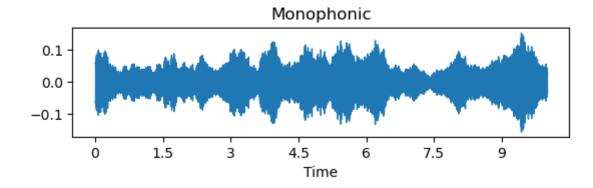
# Classify music style from audio files

• Imagine you are asked to develop a music style classification system to help a song recommendation system.

- E.g., something similar to what Spotify does
- Training data: audio files along with their music styles (e.g., classical, blues, pop)
- Prediction task: Given a new raw audio file predict the music style of in the audio.
- You can download the data from <u>MARSYAS (http://marsyas.info/downloads/datasets.html)</u>.
   You can also get it <u>from kaggle (https://www.kaggle.com/datasets/andradaolteanu/gtzandataset-music-genre-classification)</u> in the genres\_original folder.
  - Beware of the size; it is 1.2 GB.
- We'll be using librosa library for feature engineering of audio files.
- You can install librosa in your conda environment as follows:

conda install -c conda-forge librosa

### Out[17]: Text(0.5, 1.0, 'Monophonic')



### Out[18]:

0:00 / 0:00

- I have taken a subset of the above dataset with genres and stored it in music\_genres\_small
  - blues
  - classical
  - pop

- rock
- Let's extract some domain-specific features called <u>MFCC features</u>
   (<a href="https://en.wikipedia.org/wiki/Mel-frequency\_cepstrum">https://en.wikipedia.org/wiki/Mel-frequency\_cepstrum</a>) from the above subset and store it as a CSV. I am pushing this CSV in the repo.
- (You do not need to understand the feature extraction code below.)

```
data dir = "../data/music genres small/"
In [20]:
             raw audio X = np.empty(shape=(400, 1))
            raw audio X10 = np.empty(shape=(400, 10))
           3
             raw_audio_X10k = np.empty(shape=(400, 10000))
             raw_audio_y = []
             row ind = 0
           7
             for audio file in glob.glob(data dir + r"*/*.wav"):
           8
          9
                 y, sr = librosa.load(audio file, mono=True, duration=30)
                 mfcc = librosa.feature.mfcc(y=y, sr=sr)
          10
          11
                 chroma stft = librosa.feature.chroma stft(y=y, sr=sr)
                 spec cent = librosa.feature.spectral centroid(y=y, sr=sr)
          12
          13
                 spec bw = librosa.feature.spectral bandwidth(y=y, sr=sr)
          14
                 rolloff = librosa.feature.spectral rolloff(y=y, sr=sr)
          15
                 zcr = librosa.feature.zero crossing rate(y)
          16
                 filename = ntpath.basename(audio_file)
          17
                 label = filename.split(".")[0]
          18
          19
                 data.setdefault("audio_file", []).append(filename)
                 data.setdefault("label", []).append(label)
          20
          21
                 data.setdefault("chroma_stft", []).append(np.mean(chroma_stft))
          22
                 data.setdefault("spec_cent", []).append(np.mean(spec_cent))
          23
                 data.setdefault("spec_bw", []).append(np.mean(spec_bw))
                 data.setdefault("rolloff", []).append(np.mean(rolloff))
          24
                 data.setdefault("zcr", []).append(np.mean(zcr))
          25
          26
          27
                 # Get mfcc features
          28
                 feat prefix = "mfcc"
          29
                 ind = 1
          30
                 for feat in mfcc:
          31
                     key = feat prefix + str(ind)
          32
                     data.setdefault(key, []).append(np.mean(feat))
          33
                     ind += 1
          34
                 try:
          35
                     raw_audio_X[row_ind] = np.mean(y)
          36
                     raw audio X10[row ind] = y[:10]
          37
                     raw audio X10k[row ind] = y[:10000]
          38
                     raw audio y.append(label)
          39
                 except:
                     print("Broadcasting problem with file %s" % (audio file))
          40
          41
                 row ind += 1
          42
          43
             df = pd.DataFrame(data)
             df.to csv("../data/genres/music genre.csv", index=False)
```

If we just pass raw audio data to an ML model.

 We could just take the mean of the audio time series which won't be much meaningful in each case.

### Out[21]:

	fit_time	score_time	test_score	train_score
0	0.000849	0.000189	0.250000	0.261719
1	0.000447	0.000114	0.250000	0.261719
2	0.000440	0.000105	0.265625	0.257812
3	0.000416	0.000105	0.265625	0.257812
4	0.000408	0.000105	0.265625	0.257812

If we just pass raw audio data to an ML model.

- We could just take the mean of the audio time series which won't be much meaningful in each case...
- Or we could take the beginning of the series... This is better but still not great at all.

```
In [22]:
```

```
1
  raw audio y = np.asarray(raw audio y)
2
   results = {}
3
   for X in [raw audio X10, raw audio X10k]:
       X train, X test, y train, y test = train test split(
           X, raw_audio_y, test_size=0.20, random state=111
5
6
7
       lr = LogisticRegression(solver="liblinear")
       res = pd.DataFrame(cross validate(lr, X train, y train, return trai
8
9
       print(res)
10
       print(np.mean(res['test score']))
11
```

```
fit time score time test score train score
0 0.001102
              0.000164
                          0.312500
                                       0.398438
1 0.000793
              0.000112
                          0.312500
                                       0.371094
2 0.000748
              0.000105
                          0.343750
                                       0.359375
3 0.000740
              0.000103
                          0.296875
                                       0.351562
4 0.000755
              0.000105
                          0.375000
                                       0.386719
0.328125
  fit_time score_time test_score train_score
0 1.450364
              0.000750
                          0.312500
                                            1.0
1 1.323437
              0.000709
                          0.390625
                                            1.0
2 1.368735
              0.000692
                          0.328125
                                            1.0
3 1.395656
              0.000719
                          0.359375
                                            1.0
4 1.375528
              0.000713
                          0.312500
                                            1.0
0.340625
```

Let's try it with standard domain-specific MFCC features.

### Out[23]:

	TIT_TIME	score_time	test_score	train_score
0	0.008478	0.000660	0.703125	0.914062
1	0.008674	0.000644	0.796875	0.906250
2	0.008776	0.000586	0.781250	0.898438
3	0.007765	0.000571	0.765625	0.890625
4	0.008103	0.000565	0.781250	0.898438

- Much better results with domain-specific features!!
- · You could improve it further with more careful feature engineering.

### **Summary**

- Feature engineering is finding the useful representation of the data that can help us effectively solve our problem.
- We looked at commonly used features in text data
  - Bag of word features
  - N-gram features
  - Part-of-speech features
  - Classify music style from audio files

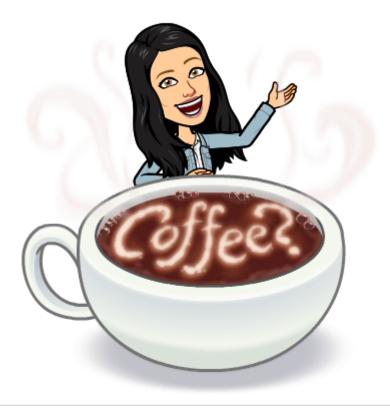
# Feature engineering

- The best features are application-dependent.
- It's hard to give general advice. But here are some guidelines.
  - Ask the domain experts.
  - Go through academic papers in the discipline.
  - Often have idea of right discretization/standardization/transformation.
  - If no domain expert, cross-validation will help.
- If you have lots of data, use deep learning methods.

The algorithms we used are very standard for Kagglers ... We spent most of our efforts in feature engineering...

- Xavier Conort, on winning the Flight Quest challenge on Kaggle

# Break (5 min)



# Feature selection: Introduction and motivation

- With so many ways to add new features, we can increase dimensionality of the data.
- More features means more complex models, which means increasing the chance of overfitting.

### What is feature selection?

• Find the features (columns) X that are important for predicting y, and remove the features that aren't

• Given 
$$X = \begin{bmatrix} x_1 & x_2 & \dots & x_n \\ & & & \end{bmatrix}$$
 and  $y = \begin{bmatrix} \\ \\ \end{bmatrix}$ , find the columns  $1 \le j \le n$  in  $X$  that are important for predicting  $y$ .

### Why feature selection?

- Interpretability: Models are more interpretable with fewer features. If you get the same performance with 10 features instead of 500 features, why not use the model with smaller number of features?
- Computation: Models fit/predict faster with fewer columns.
- Data collection: What type of new data should I collect? It may be cheaper to collect fewer columns.
- Fundamental tradeoff: Can I reduce overfitting by removing useless features?

Feature selection can often result in better performing (less overfit), easier to understand, and faster model.

# How do we carry out feature selection?

- · There are a number of ways.
- · You could use domain knowledge to discard features.
- We are briefly going to look at two automatic feature selection methods from sklearn:
  - Model-based selection
  - Recursive feature elimination
  - Forward selection
- · Very related to looking at feature importances.

```
In [24]:
            from sklearn.datasets import load breast cancer
          2
          3 cancer = load breast cancer()
          4 | X train, X test, y train, y test = train test split(
          5
                 cancer.data, cancer.target, random state=0, test size=0.5
           6
In [25]:
          1 X train.shape
Out[25]: (284, 30)
In [26]:
          1 pipe lr all feats = make pipeline(StandardScaler(), LogisticRegression(
          2 pipe_lr_all_feats.fit(X_train, y_train)
          3 pd.DataFrame(
                 cross validate(pipe lr all feats, X train, y train, return train sc
            ).mean()
Out[26]: fit time
                        0.002101
         score time
                        0.000177
         test score
                        0.968233
         train_score
                        0.987681
         dtype: float64
```

### **Model-based selection**

Use a supervised machine learning model to judge the importance of each feature.

- · Keep only the most important ones.
- Supervised machine learning model used for feature selection can be different that the one used as the final estimator.
- Use a model which has some way to calculate feature importances.
- To use model-based selection, we use SelectFromModel transformer.
- It selects features which have the feature importances greater than the provided threshold.
- Below I'm using RandomForestClassifier for feature selection with threahold "median" of feature importances.
- · Approximately how many features will be selected?

We can put the feature selection transformer in a pipeline.

```
In [28]:
             pipe lr model based = make pipeline(
           1
                 StandardScaler(), select_rf, LogisticRegression(max_iter=1000)
           2
           3
           4
             pd.DataFrame(
                 cross validate(pipe lr model based, X train, y train, return train
             ).mean()
Out[28]: fit time
                         0.072111
         score time
                         0.005723
         test score
                         0.950564
         train score
                         0.974480
         dtype: float64
```

Out[29]: (284, 15)

Similar results with only 15 features instead of 30 features.

# Recursive feature elimination (RFE)

- · Build a series of models
- At each iteration, discard the least important feature according to the model.
- · Computationally expensive
- · Basic idea
  - fit model
  - find least important feature

- remove
- iterate.

# **RFE** algorithm

- 1. Decide *k*, the number of features to select.
- 2. Assign importances to features, e.g. by fitting a model and looking at coef\_ or feature\_importances\_.
- 3. Remove the least important feature.
- 4. Repeat steps 2-3 until only *k* features are remaining.

Note that this is **not** the same as just removing all the less important features in one shot!

```
In [30]: 1 scaler = StandardScaler()
2 X_train_scaled = scaler.fit_transform(X_train)
```

```
from sklearn.feature_selection import RFE
In [31]:
          1
          2
            # create ranking of features
          3
            rfe = RFE(LogisticRegression(), n_features_to_select=5)
             rfe.fit(X_train_scaled, y_train)
          7
             print(rfe.ranking_)
            pd.DataFrame({
          8
                 'feature': list(cancer.feature_names),
          9
         10
                 'rank': rfe.ranking_
         11
            })
         [16 12 19 13 23 20 10 1 9 22 2 25 5 7 15 4 26 18 21 8 1 1
                                                                           1 6
          14 24 3 1 17 11]
```

### Out[31]:

	feature	rank
0	mean radius	16
1	mean texture	12
2	mean perimeter	19
3	mean area	13
4	mean smoothness	23
5	mean compactness	20
6	mean concavity	10
7	mean concave points	1
8	mean symmetry	9
9	mean fractal dimension	22
10	radius error	2
11	texture error	25
12	perimeter error	5
13	area error	7
14	smoothness error	15
15	compactness error	4
16	concavity error	26
17	concave points error	18
18	symmetry error	21
19	fractal dimension error	8
20	worst radius	1
21	worst texture	1
22	worst perimeter	1
23	worst area	6
24	worst smoothness	14
25	worst compactness	24
26	worst concavity	3
27	worst concave points	1
28	worst symmetry	17
29	worst fractal dimension	11

Question: what was the first feature to be eliminated? And the last?

```
In [ ]:
In [32]:
                        1 print(rfe.support_)
                     [False False False
                       False False False False False False True True True False
                       False False True False False
                        1 print("selected features: ", cancer.feature names[rfe.support ])
In [33]:
                     selected features: ['mean concave points' 'worst radius' 'worst texture'
                      'worst perimeter'
                        'worst concave points']

    How do we know what value to pass to n features to select?

    Use RFECV which uses cross-validation to select number of features.

                        1 from sklearn.feature selection import RFECV
In [34]:
                        3 rfe_cv = RFECV(LogisticRegression(max_iter=2000), cv=10)
                        4 rfe_cv.fit(X_train_scaled, y_train)
                        5 print(rfe_cv.support_)
                        6 print(cancer.feature names[rfe cv.support ])
                     [False True False True False True True False True False
                         True True False True False False True True True True True
                       False False True True False True]
                     ['mean texture' 'mean area' 'mean concavity' 'mean concave points'
                        'mean symmetry' 'radius error' 'perimeter error' 'area error'
                        'compactness error' 'fractal dimension error' 'worst radius'
                        'worst texture' 'worst perimeter' 'worst area' 'worst concavity'
                        'worst concave points' 'worst fractal dimension']
In [35]:
                        1 rfe pipe = make pipeline(
                                       StandardScaler(),
                        3
                                       RFECV(LogisticRegression(max iter=2000), cv=10),
                                       RandomForestClassifier(n estimators=100, random state=42),
                        4
                        5
                        7 pd.DataFrame(cross_validate(rfe_pipe, X_train, y_train, return_train_sc
Out[35]: fit time
                                                       0.491919
                     score time
                                                       0.003431
                     test score
                                                       0.943609
                     train score
                                                       1.000000
                     dtype: float64
```

- Slow because there is cross validation within cross validation
- No improvement in scores (it decreases a bit) compared to all features on this toy case

### Search and score

- Define a **scoring function** f(S) that measures the quality of the set of features S.
- Now **search** for the set of features *S* with the best score.

### General idea of search and score methods

- Example: Suppose you have three features: *A*, *B*, *C* 
  - Compute **score** for  $S = \{\}$
  - Compute **score** for  $S = \{A\}$
  - Compute **score** for  $S = \{B\}$
  - Compute **score** for  $S = \{C\}$
  - Compute **score** for  $S = \{A, B\}$
  - Compute **score** for  $S = \{A, C\}$
  - Compute **score** for  $S = \{B, C\}$
  - Compute **score** for  $S = \{A, B, C\}$
- ullet Return S with the best score.
- · How many distinct combinations we have to try out?

## Forward or backward selection

- Also called wrapper methods
- · Shrink or grow feature set by removing or adding one feature at a time
- Makes the decision based on whether adding/removing the feature improves the CV score or not

```
candidates
                                                     selected
iteration
               current round
                                                                   best
                                                      features
                                                                   Score (ervor
               scores
                                  \{x_1, x_2, x_3, x_4\}
                                                        3 3
            score (x1) = 0.40
  1.
                                                                     \infty
           Score (x2) = 0.39
          Score (x3)= 0.43
         1/ Score (x4)= 0.30
 2.
       Score(x1,x4) = 0.35
                                                        {x4}
                                                                      0.30
                                   \{x_1, x_2, x_3\}
     V Score (x2, x4) = 0.28
         score (x3,x4) = 0.4
                                                        \{x_4, x_2\}
                                                                     0.28
       Score (x1, x4, x2) = 0.29 {x1, x3}
3
        Score (x3, x4, x2) = 0.30
           No score is less than the best score (error) so STOP.
```

```
In [36]:
             from sklearn.feature selection import SequentialFeatureSelector
           1
           2
           3
             pipe_forward = make_pipeline(
           4
                  StandardScaler(),
           5
                  SequentialFeatureSelector(LogisticRegression(max iter=1000), direct
                 RandomForestClassifier(n estimators=100, random state=42),
           6
           7
             pd.DataFrame(
           9
                  cross_validate(pipe_forward, X_train, y_train, return_train_score=T
          10
             ).mean()
Out[36]: fit time
                         2.154436
         score time
                         0.003376
         test score
                         0.933020
```

score\_time 0.003376 test\_score 0.933020 train\_score 1.000000 dtype: float64

```
In [37]:
             pipe forward = make pipeline(
                 StandardScaler(),
           2
           3
                 SequentialFeatureSelector(
                     LogisticRegression(max iter=1000), direction="backward", n feat
           5
           6
                 RandomForestClassifier(n estimators=100, random state=42),
           7
           8
             pd.DataFrame(
                 cross validate(pipe forward, X train, y train, return train score=T
           9
          10
             ).mean()
```

```
Out[37]: fit_time 2.720003
score_time 0.003380
test_score 0.950627
train_score 1.000000
dtype: float64
```

### Other ways to search

- · Stochastic local search
  - Inject randomness so that we can explore new parts of the search space
  - Simulated annealing
  - Genetic algorithms

# Warnings about feature selection

- A feature's relevance is only defined in the context of other features.
  - Adding/removing features can make features relevant/irrelevant.
- If features can be predicted from other features, you cannot know which one to pick.
- · Relevance for features does not have a causal relationship.
- · Don't be overconfident.
  - The methods we have seen probably do not discover the ground truth and how the world really works.
  - They simply tell you which features help in predicting  $y_i$  for the data you have.

# (Optional) Problems with feature selection

- The term 'relevance' is not clearly defined.
- · What things can go wrong with feature selection?
- Attribution: From CPSC 340.

### Example: Is "Relevance" clearly defined?

 Consider a supervised classification task of predicting whether someone has particular genetic variation (SNP)

sex	biological dad	biological mom
F	0	1
M	1	0
F	0	0
F	1	1

SNP
1
0
0
1

• True model: You almost have the same value as your biological mom.

- True model: You almost have the same value for SNP as your biological mom.
  - (SNP = biological mom) with very high probability
  - (SNP != biological mom) with very low probability



- What if "mom" feature is repeated?
- Should we pick both? Should we pick one of them because it predicts the other?
- Dependence, collinearity for linear models
  - If a feature can be predicted from the other, don't know which one to pick.

### Is "Relevance" clearly defined?

- What if we add (maternal) "grandma" feature?
- Is it relevant?
  - We can predict SNP accurately using this feature
- · Conditional independence
  - But grandma is irrelevant given biological mom feature
  - Relevant features may become irrelevant given other features

sex	biological dad	biological mom	grandma	SNP
F	0	1	1	1
M	1	0	0	О
F	0	0	0	О
F	1	1	1	1

### Is "Relevance" clearly defined?

- What if we do not know biological mom feature and we just have grandma feature
- It becomes relevant now.
  - Without mom feature this is the best we can do.
  - Features can become relevant due to missing information

sex	biological dad	grandma
F	0	1
M	1	0
F	0	0
F	1	1

SNP
1
0
О
1

- Are there any relevant features now?
- They may have some common maternal ancestor.
- What if mom likes dad because they share SNP?
- General problem (Confounding)
  - Hidden features can make irrelevant features relevant.

sex	biological dad
F	0
M	1
F	0
F	1

### Is "Relevance" clearly defined?

- Now what if we have "sibling" feature?
- The feature is relevant in predicting SNP but not the cause of SNP.
- General problem (non causality)
  - the relevant feature may not be causal

sex	biological dad	sibling
F	О	1
M	1	0
F	O	0
F	1	1

SNP
1
0
0
1

- What if you are given "baby" feature?
- Now the sex feature becomes relevant.
  - "baby" feature is relevant when sex == F
- General problem (context specific relevance)
  - adding a feature can make an irrelevant feature relevant

sex	biological dad	baby
F	O	1
M	1	1
F	O	0
F	1	1

SNP
1
0
0
1

### Warnings about feature selection

- A feature is only relevant in the context of other features.
  - Adding/removing features can make features relevant/irrelevant.
- Confounding factors can make irrelevant features the most relevant.
- If features can be predicted from other other features, you cannot know which one to pick.
- Relevance for features does not have a causal relationship.
- · Is feature selection completely hopeless?
  - It is messy but we still need to do it. So we try to do our best!

### General advice on finding relevant features

- Try forward selection.
- Try other feature selection methods (e.g., RFE, simulated annealing, genetic algorithms)
- Talk to domain experts; they probably have an idea why certain features are relevant.
- · Don't be overconfident.
  - The methods we have seen probably do not discover the ground truth and how the world really works.
  - They simply tell you which features help in predicting y<sub>i</sub>.

### **Relevant resources**

- Genome-wide association study (https://en.wikipedia.org/wiki/Genomewide association study)
- sklearn feature selection (https://scikit-learn.org/stable/modules/feature\_selection.html)
- <u>PyData: A Practical Guide to Dimensionality Reduction Techniques</u>
   (<a href="https://www.youtube.com/watch?v=ioXKxulmwVQ">https://www.youtube.com/watch?v=ioXKxulmwVQ</a>)

# True/False questions for class discussion

- 1. Simple association-based feature selection approaches do not take into account the interaction between features.
- 2. You can carry out feature selection using linear models by pruning the features which have very small weights (i.e., coefficients less than a threshold).
- 3. Forward search is guaranteed to find the best feature set.
- 4. The order of features removed given by rfe.ranking\_ is the same as the order of original feature importances given by the model.

In [ ]:

1